



>>Entry Name: 3,5-Dibromobenzoic acid

CAS Registry Number: 618-58-6

Molecular Formula: $C_7H_4Br_2O_2$

Molecular Weight: 279.915

Accurate Mass: 277.897802

Percentage Composition: C 30.04%; H 1.44%; Br 57.09%; O 11.43%

Physical Description: Needles or leaflets

Melting Point: Mp 219-220°

Other Data: Sublimes

Hazard & Toxicity: LD₅₀ (mus, ipr) 562 mg/kg

Aldrich: 41152-3

Fluka: 33960

>>Derivative: Me ester

CAS Registry Number: 51329-15-8

Molecular Formula: $C_8H_6Br_2O_2$

Molecular Weight: 293.942

Accurate Mass: 291.913452

Percentage Composition: C 32.69%; H 2.06%; Br 54.37%; O 10.89%

Physical Description: Needles

Melting Point: Mp 63°

>>Derivative: Et ester

CAS Registry Number: 67973-33-5

Molecular Formula: $C_9H_8Br_2O_2$

Molecular Weight: 307.969

Accurate Mass: 305.929102

Percentage Composition: C 35.10%; H 2.62%; Br 51.89%; O 10.39%

Melting Point: Mp 58°

>>Derivative: Chloride

Molecular Formula: $C_7H_3Br_2ClO$

Molecular Weight: 298.361

Accurate Mass: 295.863914

Percentage Composition: C 28.18%; H 1.01%; Br 53.56%; Cl 11.88%; O 5.36%

Physical Description: Needles

Melting Point: Mp 41-42°

Boiling Point: Bp₄₅ 189°

>>Derivative: Amide

Molecular Formula: $C_7H_5Br_2NO$

Molecular Weight: 278.931

Accurate Mass: 276.913786

Percentage Composition: C 30.14%; H 1.81%; Br 57.29%; N 5.02%; O 5.74%

Physical Description: Needles

Melting Point: Mp 187°

>>Derivative: Nitrile

Synonym(s): 1,3-Dibromo-5-cyanobenzene

CAS Registry Number: 97165-77-0

Molecular Formula: $C_7H_3Br_2N$

Molecular Weight: 260.915

Accurate Mass: 258.903221

Percentage Composition: C 32.22%; H 1.16%; Br 61.25%; N 5.37%

Physical Description: Needles

Melting Point: Mp 97°

Other Data: Sublimes

References: